In the Claims

Claims 1-179 (Canceled).

Claim 180 (Currently Amended): A method of identifying crystalline salts of a small molecule pharmaceutical using a system comprising a series of integrated modules, or workstations, comprising:

(a) preparing and identifying an array of at least 96 samples in tubes and support plates or in sample well plates using an automated dispensing apparatus directed by a work list generated by formulation software, said work list allowing a file to be used as a process command rather than discrete programmed steps, and dispensing components into sample tubes or sample wells with a sample generation module, wherein each sample contains less than about 100 milligrams of said small molecule pharmaceutical, and each sample differs with respect to at least one of:

(i) the amount or concentration of the small molecule pharmaceutical;

(ii) an identity of one or more of a solvent, acid or base; or

(iii) an amount or concentration of one or more of a solvent, acid or base;

(b) sealing said samples;

(c) processing said samples comprising heating said samples in a sample incubation module to a temperature (T1), analyzing said samples for the presence of undissolved solids using visual analysis, cooling said samples to a final temperature (T2), wherein at least one of the processed samples comprises a crystalline salt form of the small molecule pharmaceutical;

(d) analyzing the processed array of samples comprising detecting crystalline solid formation in said samples using visual analysis, measuring a property for each crystalline solid and using the results of said measuring to group samples containing similar crystalline salt polymorphs, hydrates and solvates that belong to the same crystal family-~~using~~ informatics.

Claim 181 (Currently Amended): The method of claim 180, comprising the further spectroscopic, diffractometric, or thermal analysis of at least one representative of each crystal family and any orphan crystals.

Claim 182 (Previously Presented): The method of claim 180, comprising the addition of said samples to tubes in a support plate.

Claim 183 (Previously Presented): The method of claim 182, wherein said tubes are glass tubes and said support plate is a metal support plate.

Claim 184 (Previously Presented): The method of claim 182, comprising sealing said tubes with a cap.

Claim 185 (Withdrawn): The method of claim 180, wherein said array comprises at least 1000 samples.

Claim 186 (Canceled):

Claim 187 (Previously Presented): The method of claim 180, comprising the dispensing of components by a liquid handling system with pipette tips having septum-piercing capability.

Claim 188 (Previously Presented): The method of claim 180, wherein said sample contains less than 1 milligram of said small molecule pharmaceutical.

Claim 189 (Canceled).

Claim 190 (Previously Presented): The method of claim 180, wherein said processing further comprises the quenching of the crystallization process by removing solvent from the samples.

Claim 191 (Previously Presented): The method of claim 180, wherein said processing further comprises adding a non-solvent to said samples.

Claim 192 (Previously Presented): The method of claim 180, wherein said processing further comprises evaporating solvent from said samples.

Claim 193 (Previously Presented): The method of claim 184, comprising the piercing of said cap and aspiration of fluid from said samples.

Claim 194 (Withdrawn): The method of claim 180, comprising analyzing said array of samples with a polarized light filter apparatus.

Claim 195 (Withdrawn): The method of claim 180, wherein the small molecule pharmaceutical has previously evaded crystallization.

Claim 196 (Withdrawn): The method of claim 180, wherein the crystalline salt identified in said processed samples is an additional polymorph of small molecule pharmaceutical previously known as a monomorphic compound.

Claim 197 (Withdrawn): The method of claim 180, wherein said visual analysis is used as a filtering means to reduce the numbers of samples that will ultimately undergo in-depth analysis.

Claim 198 (Previously Presented): The method of claim 180, wherein said grouped samples comprise a category selected from the group consisting of: a) samples containing no precipitate; b) samples with a single polymorph; c) samples with a polymorph mixture; d) samples with amorphous forms of said small molecule pharmaceutical; and e) samples with mixtures of categories b-d.

Claim 199 (Previously Presented): The method of claim 180, further comprising analyzing said samples for at least one additional property, wherein said property is a chemical, structural or physical property.

Claim 200 (Previously Presented): The method of claim 180, wherein said small molecule pharmaceutical is a known compound.

Claim 201 (Withdrawn): The method of claim 180, wherein said small molecule pharmaceutical is an unknown compound.

Claim 202 (Withdrawn): The method of claim 180, wherein said array comprises at least 1 sub-array.

Claim 203 (Withdrawn): The method of claim 180, wherein said array comprises at least 1 sub-array with at least 24 samples.

Claim 204 (Previously Presented): The method of claim 180, wherein an individual sample within said array is subjected to processing methods that are different from the processing methods to which another sample is subjected.

Claim 205 (Withdrawn): The method of claim 204, wherein said individual sample is subjected to processing methods comprising adjusting the solvent removal rate.

Claim 206 (Withdrawn): The method of claim 204, wherein said individual sample is subjected to processing methods comprising introducing a nucleation event.

Claim 207 (Previously Presented): The method of claim 204, wherein said individual sample is subjected to processing methods comprising adding one or more additional components.

Claim 208 (Withdrawn): The method of claim 204, wherein said individual sample is subjected to processing methods comprising introducing a precipitation event.

Claim 209 (Withdrawn): The method of claim 204, wherein said individual sample is subjected to processing methods comprising adjusting the solvent composition.

Claim 210 (Withdrawn): The method of claim 204, wherein said individual sample is subjected to processing methods comprising adjusting or controlling evaporation of the solvent.

Claim 211 (Withdrawn): The method of claim 204, wherein said individual sample is subjected to processing methods comprising adding a non-solvent.

Claim 212 (Withdrawn): The method of claim 180, wherein said array comprises sub-arrays, and wherein an individual sample within a sub-array is subjected to processing methods that are different from the processing methods to which another sample within the sub-array is subjected.

Claim 213 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising adjusting the solvent removal rate.

Claim 214 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising introducing a nucleation event.

Claim 215 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising adding one or more additional components.

Claim 216 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising introducing a precipitation event.

Claim 217 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising adjusting the solvent composition.

Claim 218 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising adjusting or controlling evaporation of the solvent.

Claim 219 (Withdrawn): The method of claim 212, wherein said individual sample is subjected to processing methods comprising adding a non-solvent.

Claim 220 (Withdrawn): The method of claim 180, wherein said array comprises sub-arrays, and wherein an individual sub-array is subjected to processing methods that are different from the processing methods to which another sub-array is subjected.

Claim 221 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising adjusting the solvent removal rate.

Claim 222 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising introducing a nucleation event.

Claim 223 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising adding one or more additional components.

Claim 224 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising introducing a precipitation event.

Claim 225 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising adjusting the solvent composition.

Claim 226 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising adjusting or controlling evaporation of the solvent.

Claim 227 (Withdrawn): The method of claim 220, wherein said individual sub-array is subjected to processing methods comprising adding a non-solvent.

Claim 228 (Previously Presented): The method of claim 180, wherein said small molecule pharmaceutical has a molecular weight less than about 1000 g/mol.

Claim 229 (Canceled).

Claim 230 (Previously Presented): The method of claim 180, wherein the amount of said small molecule pharmaceutical in each sample is less than about 100 micrograms.

Claim 231 (Previously Presented): The method of claim 180, wherein the amount of said small molecule pharmaceutical in each sample is less than about 100 nanograms.

Claim 232 (Previously Presented): The method of claim 180, wherein the total volume of each sample is between 100-250 μl.

Claim 233 (Previously Presented): The method of claim 184, wherein said cap can be pierced with a standard syringe needle and fluid aspirated through the syringe tip to remove solvent from the sample.

Claim 234 (Previously Presented): The method of claim 180, wherein one or more samples differ from one or more other samples with respect to the amount or concentration of the small molecule pharmaceutical.

Claim 235 (Previously Presented): The method of claim 180, wherein one or more samples differ from one or more other samples with respect to the identity of one or more of a solvent.

Claim 236 (Withdrawn): The method of claim 180, wherein said small molecule pharmaceutical is added to a series of different solvents ranging in polarity from extremely polar to non-polar.

Claim 237 (Withdrawn): The method of claim 180, wherein mixed solvents are used to change the thermodynamic activity of one of the solvents independent of temperature.

Claim 238 (Withdrawn): The method of claim 180, wherein one or more samples differ from one or more other samples with respect to the amount or concentration of one or more of an acid.

Claim 239 (Withdrawn): The method of claim 238, wherein said one or more of an acid are those that form succinate, chloride, malate, or stearate salts with a basic compound.

Claim 240 (Withdrawn): The method of claim 238, wherein said acid are those that form maleate, citrate, tartrate, or mesylate salts with a basic compound.

Claim 241 (Withdrawn): The method of claim 238, wherein said acid are those that form succinate, acetate, chloride or mesylate salts with a basic compound.

Claim 242 (Withdrawn): The method of claim 238, wherein said acid are those that form chloride, malate, maleate, or mesylate salts with a basic compound.

Claim 243 (Withdrawn): The method of claim 238, wherein said acid are those that form succinate, stearate, citrate or tartrate salts with a basic compound.

Claim 244 (Withdrawn): The method of claim 238, wherein said acid are those that form acetate, succinate, mesylate or stearate salts with a basic compound.

Claim 245 (Withdrawn): The method of claim 238, wherein said acid are those that form benzenesulfonate, malate, mesylate or succinate salts with a basic compound.

Claim 246 (Previously Presented): The method of claim 180, wherein one or more samples differ from one or more other samples with respect to the identity of one or more of a base.

Claims 247-248 (Canceled).

Claim 249 (Previously Presented): The method of claim 180, wherein said components comprise an additive that affects polymorphic form.

Claims 250-257 (Canceled).

Claim 258 (Previously Presented): The method of claim 199, wherein the physical property screened is solubility.

Claim 259 (Withdrawn): The method of claim 199, wherein the physical property screened is dissolution.

Claim 260 (Withdrawn): The method of claim 199, wherein the physical property screened is compressibility.

Claim 261 (Withdrawn): The method of claim 199, wherein the physical property screened is compactibility.

Claim 262 (Withdrawn): The method of claim 199, wherein the physical property screened is melting point.

Claim 263 (Withdrawn): The method of claim 199, wherein the physical property screened is resistance to absorption of ambient moisture.

Claim 264 (Withdrawn): The method of claim 199, wherein the physical property screened is bioavailability.

Claim 265 (Withdrawn): The method of claim 199, wherein the structural property screened is surface to volume ratio.

Claim 266 (Withdrawn): The method of claim 199, wherein the structural property screened is degree of agglomeration.

Claim 267 (Withdrawn): The method of claim 199, wherein the structural property screened is porosity.

Claim 268 (Withdrawn): The method of claim 199, wherein the structural property screened is particle size.

Claim 269 (Withdrawn): The method of claim 199, wherein the structural property screened is particle size distribution.

Claim 270 (Withdrawn): The method of claim 199, wherein the chemical property screened is chemical stability.

Claim 271 (Withdrawn): The method of claim 199, wherein the structural property screened is resistance to chemical reactions induced by heat.

Claim 272 (Withdrawn): The method of claim 199, wherein the structural property screened is resistance to chemical reactions induced by ultraviolet light.

Claim 273 (Withdrawn): The method of claim 199, wherein the structural property screened is resistance to chemical reactions induced by moisture.

Claim 274 (Withdrawn): The method of claim 199, wherein the structural property screened is resistance to chemical reactions between components.

Claim 275 (Withdrawn): The method of claim 199, wherein the structural property screened is resistance to chemical reactions induced by oxygen.

Claim 276 (Currently Amended): The method of claim 180, wherein the processed samples are analyzed by ~~machine vision technology~~ a charge coupled camera.

Claim 277 (Withdrawn): The method of claim 180, wherein the processed samples are analyzed by video-optical microscopy.

Claim 278 (Withdrawn): The method of claim 180, wherein the processed samples are analyzed by image analysis.

Claim 279 (Withdrawn): The method of claim 189, wherein the processed samples are analyzed by polarized light analysis.

Claim 280 (Withdrawn): The method of claim 180, wherein the processed samples are analyzed by near field scanning optical microscopy.

Claim 281 (Withdrawn): The method of claim 180, wherein the processed samples are analyzed by far field scanning optical microscopy.

Claim 282 (Withdrawn): The method of claim 180, wherein the processed samples are analyzed by atomic-force microscopy.

Claim 283 (Withdrawn): The method of claim 180, wherein the processed samples are analyzed by micro-thermal analysis.

Claim 284 (Withdrawn): The method of claim 180, comprising analyzing the crystalline salt form by infrared spectroscopy.

Claim 285 (Withdrawn): The method of claim 180, comprising analyzing the crystalline salt form by near infrared spectroscopy.

Claim 286 (Previously Presented): The method of claim 180, comprising analyzing the crystalline salt form by Raman spectroscopy.

Claims 287-294 (Canceled).

Claim 295 (Previously Presented): The method of claim 180, wherein said crystalline salt form is a solvate.

Claim 296 (Withdrawn): The method of claim 180, wherein said crystalline salt form is a desolvated solvate.

Claim 297 (Withdrawn): The method of claim 180, wherein said crystalline salt form is, a clathrate.

Claim 298 (Withdrawn): The method of claim 180, wherein said crystalline salt form is an inclusion.

Claim 299 (Previously Presented): The method of claim 180, wherein said system comprises a sample incubation and sample detection module.

Claim 300 (Previously Presented): The method of claim 180, wherein data collected is used to identify occurrence of conditions that define occurrence domains that will give rise to a specific crystal form.

Claim 301 (Canceled).

Claim 302 (Currently Amended): A method of identifying crystalline salts of a small molecule pharmaceutical using a system comprising a series of integrated modules, or workstations, comprising:

(a) preparing and identifying an array of at least 96 samples in tubes and support plates or in sample well plates using an automated dispensing apparatus directed by a work list generated by formulation software, said work list allowing a file to be used as a process command rather than discrete programmed steps, and dispensing components into sample tubes or sample wells with a sample generation module, wherein each sample contains less than about 100 milligrams of said small molecule pharmaceutical, one or more of a solvent, and each sample differs with respect to at least one of:

(i) the amount or concentration of the small molecule pharmaceutical;

(ii) an amount, concentration or identity of said one or more of a solvent; or

(iii) an amount, concentration or identity of one or more of an acid or base;

(b) sealing said samples;

(c) processing said samples comprising evaporating solvent from said samples wherein at least one of the processed samples comprises a crystalline salt form of the small molecule pharmaceutical;

(d) analyzing the processed array of samples comprising detecting crystalline solid formation in said samples using visual analysis, measuring a property for each crystalline solid and using the results of said measuring to group similar crystalline salt polymorphs, hydrates and solvates that belong to the same crystal family ~~using informatics~~.

Claim 303 (Currently Amended): A method of identifying crystalline salts of a small molecule pharmaceutical using a system comprising a series of integrated modules, or workstations, comprising:

(a) preparing and identifying an array of at least 96 samples in tubes and support plates or in sample well plates using an automated dispensing apparatus directed by a work list generated by formulation software, said work list allowing a file to be used as a process command rather than discrete programmed steps, and dispensing components into sample tubes or sample wells with a sample generation module, wherein each sample contains less than about 100 milligrams of said small molecule pharmaceutical, and each sample differs with respect to at least one of:

(i) the amount or concentration of the small molecule pharmaceutical;

(ii) an identity of one or more of a solvent, acid or base; or

(iii) an amount or concentration of one or more of a solvent, acid or base;

(b) sealing said samples;

(c) processing said samples comprising adding an antisolvent to said samples wherein at least one of the processed samples comprises a crystalline salt form of the small molecule pharmaceutical;

(d) analyzing the processed array of samples comprising detecting crystalline solid formation in said samples using visual analysis, measuring a property for each crystalline solid and using the results of said measuring to group similar crystalline salt polymorphs, hydrates and solvates that belong to the same crystal family ~~using informatics~~.

Claim 304 (Currently Amended): A method of identifying crystalline salts of a small molecule pharmaceutical comprising:

(a) preparing and identifying an array of at least 96 samples in tubes and support plates or in sample well plates using an automated dispensing apparatus directed by a work list generated by formulation software, said work list allowing a file to be used as a process command rather than discrete programmed steps, and dispensing: i) said small molecule pharmaceutical; a salt forming component; and additional components into sample tubes or sample wells with a sample generation module, wherein said array comprises at least 1 group of at least 24 samples, each sample contains less than about 100 milligrams of said small molecule pharmaceutical, and each sample differs with respect to at least one of:

(i) the amount or concentration of the small molecule pharmaceutical;

(ii) an identity of one or more of a solvent, acid or base; or

(iii) an amount or concentration of one or more of a solvent, acid or base;

(b) sealing said samples;

(c) processing said samples comprising heating said samples in a sample incubation module to a temperature (T1), analyzing said samples for the presence of undissolved solids using visual analysis, cooling said samples to a final temperature (T2), wherein at least one of the processed samples comprises a crystalline salt form of the small molecule pharmaceutical; and

(d) analyzing the processed array of samples comprising detecting crystalline solid formation in said samples using visual analysis, measuring a property for each crystalline solid and using the results of said measuring to group similar crystalline salt polymorphs, hydrates and solvates that belong to the same crystal family ~~using informatics~~.

Claim 305 (New): The method according to claim 180, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide).

Claim 306 (New): The method according to claim 180, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide); said array of at least 96 samples is prepared in glass tubes; said support plates or sample well plates is are heating/cooling blocks; said samples are grouped using Raman spectroscopy; said samples are analyzed using Raman spectroscopy;

Claim 307 (New): The method according to claim 180, wherein said samples are grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 308 (New): The method according to claim 305, wherein said small molecule pharmaceutical is grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 309 (New): The method according to claim 180, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide, which has not evaded crystallization and is a known compound; said tubes are glass vials; said support plates or sample well plates are heating/cooling blocks said automated dispensing apparatus is a Tecan Genesis with septum piercing capability; said formulation software is Matlab software; said analysis is Raman spectroscopy; said array number is at least 96 samples and wherein zero subarrays are contained within said array; said solvent, for all samples, is sodium hydroxide (NaOH); said sample difference is the amount of water between samples; said samples are grouped using Raman spectroscopy; said samples are grouped into samples containing a single polymorph; said samples are processed by cooling; said samples contain less than 100 µg; said sample volume is 100 µl; said species of components, if present, is a polymorphic form and sodium chloride (NaCl) in an aqueous solution as the additive; solubility is the physical property screened; particle size is the structural property screened; and the species of crystalline salt form is solvate.

Claim 310 (New): The method according to claim 302, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide).

Claim 311 (New): The method according to claim 302, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide); said array of at least 96 samples is prepared in glass tubes; said support plates or sample well plates is are heating/cooling blocks; said samples are grouped using Raman spectroscopy; said samples are analyzed using Raman spectroscopy.

Claim 312 (New): The method according to claim 302, wherein said samples are grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 313 (New): The method according to claim 310, wherein said small molecule pharmaceutical is grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 314 (New): The method according to claim 302, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide, which has not evaded crystallization and is a known compound; said tubes are glass vials; said support plates or sample well plates are heating/cooling blocks said automated dispensing apparatus is a Tecan Genesis with septum piercing capability; said formulation software is Matlab software; said analysis is Raman spectroscopy; said array number is at least 96 samples and wherein zero subarrays are contained within said array; said solvent, for all samples, is sodium hydroxide (NaOH); said sample difference is the amount of water between samples; said samples are grouped using Raman spectroscopy; said samples are grouped into samples containing a single

polymorph; said samples are processed by cooling; said samples contain less than 100 µg; said sample volume is 100 µl; said species of components, if present, is a polymorphic form and sodium chloride (NaCl) in an aqueous solution as the additive; solubility is the physical property screened; particle size is the structural property screened; and the species of crystalline salt form is solvate.

Claim 315 (New): The method according to claim 303, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide).

Claim 316 (New): The method according to claim 303, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide); said array of at least 96 samples is prepared in glass tubes; said support plates or sample well plates is are heating/cooling blocks; said samples are grouped using Raman spectroscopy; said samples are analyzed using Raman spectroscopy;

Claim 317 (New): The method according to claim 303, wherein said samples are grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 318 (New): The method according to claim 315, wherein said small molecule pharmaceutical is grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 319 (New): The method according to claim 303, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide, which has not evaded crystallization and is a known compound; said tubes are glass vials; said support plates or sample well plates are heating/cooling blocks said automated

dispensing apparatus is a Tecan Genesis with septum piercing capability; said formulation software is Matlab software; said analysis is Raman spectroscopy; said array number is at least 96 samples and wherein zero subarrays are contained within said array; said solvent, for all samples, is sodium hydroxide (NaOH); said sample difference is the amount of water between samples; said samples are grouped using Raman spectroscopy; said samples are grouped into samples containing a single polymorph; said samples are processed by cooling; said samples contain less than 100 μg; said sample volume is 100 μl; said species of components, if present, is a polymorphic form and sodium chloride (NaCl) in an aqueous solution as the additive; solubility is the physical property screened; particle size is the structural property screened; and the species of crystalline salt form is solvate.

Claim 320 (New): The method according to claim 304, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide).

Claim 321 (New): The method according to claim 304, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide); said array of at least 96 samples is prepared in glass tubes; said support plates or sample well plates is are heating/cooling blocks; said samples are grouped using Raman spectroscopy; said samples are analyzed using Raman spectroscopy;

Claim 322 (New): The method according to claim 304, wherein said samples are grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 323 (New): The method according to claim 320, wherein said small molecule pharmaceutical is grouped using Raman spectroscopy and said samples are analyzed using Raman spectroscopy.

Claim 324 (New): The method according to claim 304, wherein said small molecule pharmaceutical is celecoxib (4-[5-(4-methylphenyl)-3- (trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide; 4-(1,1,1-trifluoromethyl- 5-(4-methylphenyl) pyrazol-1-yl)-benzenesulfonamide, which has not evaded crystallization and is a known compound; said tubes are glass vials; said support plates or sample well plates are heating/cooling blocks said automated dispensing apparatus is a Tecan Genesis with septum piercing capability; said formulation software is Matlab software; said analysis is Raman spectroscopy; said array number is at least 96 samples and wherein zero subarrays are contained within said array; said solvent, for all samples, is sodium hydroxide (NaOH); said sample difference is the amount of water between samples; said samples are grouped using Raman spectroscopy; said samples are grouped into samples containing a single polymorph; said samples are processed by cooling; said samples contain less than 100 μg; said sample volume is 100 μl; said species of components, if present, is a polymorphic form and sodium chloride (NaCl) in an aqueous solution as the additive; solubility is the physical property screened; particle size is the structural property screened; and the species of crystalline salt form is solvate.